# Trip Report – IRSN Meetings & OECD-NEA-WPNCS Expert Group Meetings
## Paris, France, 26-30 June 2017

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### 1.0 Introduction

During 26-27 June, 2017, Brown, Rising, and Alwin visited IRSN for technical interchange meetings with the nuclear criticality safety (NCS) group at IRSN. During 28-30 June, 2017, Brown and Rising participated in the OECD-NEA-WPNCS Expert Group meetings on Advanced Monte Carlo Techniques (EGAMCT) and Uncertainty Analysis for Criticality Safety Applications (EGUACSA). Each of these meetings is summarized below.

### 2.0 IRSN-LANL meeting

### 2.1 Solution density laws

After introductions and practical matters, there was a lengthy discussion of solution density laws.

Nicolas Leclaire gave a presentation on the IRSN nitrate density laws implemented in the CRISTAL criticality calculation package. Basically, the solute concentrations must be converted into specific atom densities for use in Monte Carlo calculations. He discussed the Pitzer and isotemp laws used, and the Latec workbench that implements them. Presently no temperature dependence is included. He also discussed the volume additive law used for powders and the 300 tests that IRSN uses for validation of the density laws. (The Pitzer method is available in the SCALE code, but not in any of the setup utilities for MCNP.) Leclaire also discussed the nitrate density laws for $Pu(NO_3)$ and $UO_2(NO_3)$ described in a publication in Nuclear Technology (by J. Anno, et al) based on the PhD work of Charrin, which has a wider range than Pitzer's method and can possibly be applied past the solubility limit to heterogeneous mixtures.

Alwin gave a presentation on the current investigations of solution chemistry at LANL. Using a simple Pu-metal - water mix is conservative, using theoretical density 19.8 $g/cm^3$, but there is the question of how to quantify this conservatism. The effects of using $Pu(NO_3)_x$, where x= 3, 4, or 6, were looked at, using Whisper to examine sensitivity of K-effective to nuclear data. There are also investigations into the proper way to handle Pu-Chloride (rather than Pu-Nitrate), especially how to validate such calculations in the absence of benchmarks. Whisper results show that chloride vs. nitrate sensitivities have little effect on the selection of appropriate benchmarks, which was also confirmed for the theoretical plutonium metal-water mixture. Alwin also discussed future work, including study of aqueous Pu-Nitrate, oxidation state changes, determining the degree of conservatism, possible validation credit for nitrogen or chlorine absorption, and possible experiments with chemical analysis to collect binary data for the Pu(+3) solution system.

### 2.2 Monte Carlo code comparisons

At the time of this meeting, a proposed inter-code comparison of results from MCNP, COG, SCALE, and MORET was not funded, but IRSN is proceeding with the initial steps for the 3-year project. We discussed the plan and the initial LANL experience in comparing just LANL & SNL Monte Carlo results (both using MCNP6). Difficulties in code comparisons abound, including the specific revision to ICSBEP used for modeling benchmarks, differences in nuclear data libraries (ENDF/B-VII.1, JEFF-3.2, JEFF-3.3, and soon ENDF/B-VIII), simplified models vs. detailed models, models with and without impurities, etc.

Brown transmitted to IRSN the MCNP ENDF/B-VII.1 results for 1101 ICSBEP benchmarks used for the MCNP-Whisper methodology. It is hoped by both LANL & IRSN that this will encourage the other participants to provide their results to IRSN.

**2.3 Discussion & demonstration of clustering in Monte Carlo criticality calculations**

Brown gave a presentation on clustering in MC criticality calculations. Clustering is an artifact of the power method iteration used to solve MC eigenvalue (k-effective) problems. Eric Dumonteil (IRSN) has been investigating this for the past few years, and it is a topic of interest for the OECD EGAMCT. Brown presented his recent R&D in this area to the IRSN group in general, had detailed discussions with Dumonteil, and later in the week presented the work to EGAMCT. The summary of all of these discussions follows:

MC calculations for nuclear applications simulate particle behavior and tally event occurrences to estimate physical results. A fundamental assumption is that there is a sufficient number of particles in the simulation to cover the problem phase space. If this assumption is violated, all of the MC results are questionable and possibly incorrect. There is thus a central question of how to diagnose the <u>absence</u> of such coverage. In practice, running more particles will cure the problem, but questions remain on how many particles and how do you know that is enough. For criticality problems – eigenvalue calculations to determine the multiplication factor (*k-effective*) – MC calculations proceed using an iterative process, where neutrons produced in one cycle (i.e., generation) are used as the MC source for the next cycle. This is a basic power iteration scheme, with renormalization at the start of each cycle. Rather than scaling (as for a deterministic method), the neutron population is sampled to produce a prescribed number of neutrons, such that all cycles start with the same population count.

In MC criticality problems, even though the renormalization process is a fair game, intra-cycle correlation in the locations of the starting sites for MC trials is present, and this correlation can lead to non-physical clustering of the starting sites after many repeated iterations. Such clustering can especially occur when the number of neutrons starting each cycle is small. Essentially, a small population size and the renormalization process can induce non-physical clustering, a calculational artifact.

A series of problems was investigated to examine the issue of clustering – how to identify the problem, what problem characteristics promote the clustering, does clustering occur in "real-world" models with realistic geometry and physics, and what are possible metrics to diagnose the clustering effect. These include a simple model problem for which the exact solution is known (uniform particle distribution), a "real-world" problem from criticality safety with a large Pu nitrate solution volume, and a typical pressurized water reactor core. The calculations were run with the MCNP6 MC code, using idealized transport and data for the model problem and complete physics with detailed cross-sections for the other cases. Clustering is observed in all cases. Parameter studies demonstrate that clustering is promoted by higher material density, smaller mean-free path, larger problem size, and smaller numbers of neutrons/cycle.

Figure 1 illustrates the clustering phenomena for the model problem. In this idealized problem, the exact solution is a uniform distribution of neutrons. The MC calculations were started with the exact solution as the initial source guess, and depart from the exact solution due to clustering as the cycles proceed. Clustering is severe when there are too few neutrons/cycle and insignificant when there are many. Figure

2 shows the Shannon entropy of the neutron distribution during the cycles, with the roughness of the asymptotic behavior apparent for the cases of severe clustering. Similar results and observations will be shown for the realistic problems as well.

For most practical MC criticality calculations run today, clustering is not a concern due to the large numbers of neutrons/cycle recommended by "best practices" guidance. Since it may occur in applications with extreme conditions, however, practitioners need to be aware of clustering – when it may occur, how to diagnose it, and how to eliminate it. Code and methods developers need to develop a simple diagnostic to determine when clustering occurs.

Dumonteil discussed his work on modeling clustering by means of branching Brownian motion & traveling waves. This work has been published recently at the ANS Mathematics & Computation meeting.

**2.4 Discussion: IRSN specific questions and needs with MCNP**

There were continued discussions involving plutonium solution density laws with Leclaire/Alwin,

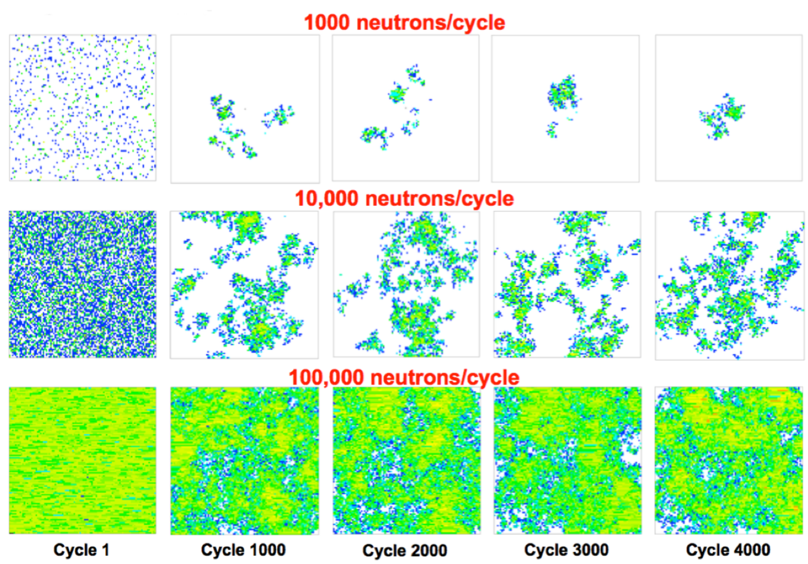


Figure 1. Neutron starting sites for model problem at various cycles, for different numbers of neutrons/cycle

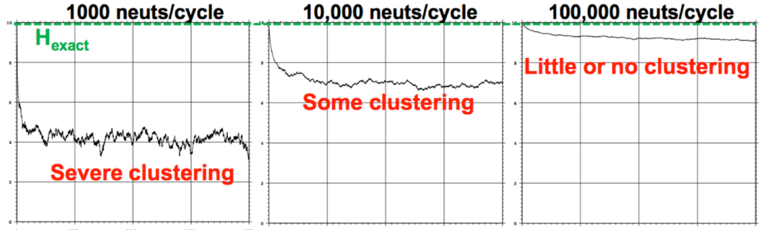


Figure 2. Shannon entropy of the neutron distribution vs cycle for the model problem, for different numbers of neutrons/cycle

including discussion of measured binary data for plutonium(+4), collected binary data applied to plutonium(+3) systems, potential measurement of plutonium(+3) binary data and specific implementation of density laws at IRSN.

Rising presented some of the MCNP class material on the unstructured mesh (UM) capability. While the use of UM is not recommended for routine k-effective calculations (due to uncertainties in preserving the volume of fissile mass), it can be very useful for shielding, dose rate, and detector calculations, and IRSN is investigating the use of UM for those applications. Rising also reviewed some of the MCNP variance reduction methods.

Alwin, Brown, & Rising presented a summary of the MCNP-Whisper methodology and gave demonstrations of its use for several practical examples based on LANL PF4 interests. The demos were well-received, and there was much IRSN interest in the application of MCNP-Whisper.

### 2.4 Discussion: IRSN methods for sensitivity-uncertainty (SU) – the Macsens tool

Alexis Jinaphanh and Frederic Fernex (IRSN) discussed the Macsens tool. This is a new IRSN capability for SU analysis. The Moret MC code can run with continuous-energy physics and produce sensitivity files (SDF files). Macsens can then read the SDF files (or even those from Scale or MCNP). It uses 44-group covariance data (as for Scale 6.1 & Whisper) and can perform GLLS analysis much like Scale/Tsurfer or the MOS portion of Whisper. Experimental correlations are included based on a report by Ivanov (IRSN report psn-exp/snc/2016-125). At present, only 6 reaction types are handled - elastic, inelastic, fission, capture, nu-bar, (nxn). (MCNP-Whisper includes 12 reaction types.)

As part of the EGUACSA benchmark Phase V, results from Moret-Macsens were found to agree very well with those from Scale/Tsunami-ip. Macsens is still a work-in-progress, but is already producing excellent results when compared to Scale/Tsunami and MCNP-Whisper.

## 3.0 OECD EGAMCT meeting

About 25 people were present at this meeting, from the US, France, UK, Germany, Finland, and a few other places. Michel-Sendis (NEA) began with a summary of the 2016 meeting. Eric Dumonteil (IRSN) is the current chair of the EG and summarized the work currently in progress: computational benchmarks on the effects of undersampling on globally distributed tallies, investigation of clustering and its impact, and the status of MC codes.

### 3.1 EGAMCT – clustering

Dumonteil presented his recent investigations into the bias on local tallies, clustering, benchmarks, and branching Brownian motion (same as presented & discussed at IRSN-LANL meeting).

Brown gave presentations on the status of the MCNP6.2 production release, the verification-validation work for NCS applications, and the R&D into clustering (as presented at the IRSN-LANL meeting).

Andrea Zoia (CEA) presented his work on investigating clustering, with a survey of power iteration in MC, fission chains, correlations, etc. He presented results for a model problem very similar to Brown's, and summarized the theory (Boltzmann and Pall-Bell equations, pair correlation functions).

Brown, Dumonteil, and Zoia all concluded that clustering is a real effect that can occur in MC criticality calculations and that we need a diagnostic tool to detect clustering. At present there is no straightforward, robust, reliable tool. There was much discussion of what to do. Brown, Dumonteil, Zoia, and Sutton (KAPL, not present) are each investigating possible diagnostic tools. Brown suggested one (expensive) possibility – perform repeated runs, with increased numbers of neutrons/cycle, until there is no apparent clustering. This would be the MC approach similar in spirit to deterministic mesh refinement.

**3.2 EGAMCT – other**

Mennerdahl (Sweden) gave a short, incoherent presentation on transport and convergence in an infinite rod model geometry.

Perfetti (ORNL) presented his recent work on searching for metrics to detect undersampling bias. A number of metrics were presented for several of the computational benchmarks. While this R&D work was necessary, it has not yet revealed a robust, reliable method for detecting undersampling.

Paul Smith (UK, ANSRS) provided a summary of the current status of the Monk MC code. Like LANL, they were still struggling to deliver a major new production release. The principal cause was "scope creep." They have been working on the fission matrix & higher modes; burnup and burnup credit; cross-section tallying; the DBRC correction for scattering kernels; CAD geometry; fractal geometry; parameter study features; Jeff-3.2 and ENDF/B-VII.1 nuclear data; and temperature effects for -40$^{o}$C problems.

**4.0 OECD EGUACSA meeting**

About 32 people were present at this meeting, from the US, France, UK, Germany, Switzerland, etc. Brad Rearden (ORNL), the chair of the EG, opened this meeting with a quick welcome and an overview of the meeting agenda. Also mentioned were the two ongoing phases (IV and V) in the EG, which ultimately received most of the attention during this meeting. At the conclusion of this meeting, Michel-Sendis (NEA) discussed the proposed restructuring of the EG and suggested that the phase IV and V efforts in this EG would likely be broken into two subgroups in the future with individual chairpersons in charge of organizing the reporting efforts of each subgroup.

**4.1 EGUACSA – code and data updates**

Ian Hill (NEA) discussed his ongoing work in producing estimated correlations between ICSBEP benchmarks within the DICE tool. While this work is essential to doing validation work properly, it is extremely difficult and time consuming to assign correlations between similar (and in many cases much older) experiments with the knowledge that is provided in the benchmark handbook. Ian stated that only a small fraction, ~2%, of the ICSBEP handbook now has some estimated correlations between similar benchmarks.

Alexander Vasiliev (PSI) presented work on using best estimate-plus-uncertainty methods for criticality safety evaluation work. This work is primarily based on making use of nuclear data adjustment techniques such as GLLS and Bayesian updating.

Alexis Jinaphanh (IRSN) gave an overview of the Macsens tool used for sensitivity/uncertainty-based criticality safety validation (similar to the presentation to the MCNP representatives at IRSN a couple of days prior). While this tool is still under development, it is already producing results as expected and will be a great tool to compare to the MCNP6/Whisper sensitivity/uncertainty-based results.

Brad Rearden (ORNL), the EGUACSA chair, deviated from the planned schedule to briefly discuss a newly created WPEC subgroup on nuclear data covariance matrices. Along with this presentation, he discussed how the covariance data has recently evolved and how major changes to this covariance data cause significant differences in the sensitivity/uncertainty-based criticality safety evaluation results. This could be a cause for concern, but because the covariance data is in its early developmental stages relative to the historical nuclear data evaluation work, and is generally conservatively estimated, significant changes to nuclear data covariance matrices are expected for some time.

### 4.2 EGUACSA – Phase IV calculation of correlations

Maik Stuke (GRS) presented the preliminary summary of results from the various participants in this phase. The discussion primarily focused on the current draft of the report where participants were tasked with estimating correlations between benchmarks used in the study. It seemed that the status of the report was temporarily on hold due to some peculiar results from one of the participants, Mennerdahl (Sweden). While it is important to include all participants' results in the final report, the consensus was that they would like to understand the source of the peculiar results and address these discrepancies in the write-up prior to finalizing the work.

### 4.3 EGUACSA – Phase V MOX applications, prediction of bias

Carmouze and Santamaria (CEA) opened the discussion on the phase V study by laying out the objectives of this work and some of the Tripoli initial results. Briefly, the CEA proposed 15 MOX application cases that were to be used in a blind study of bias prediction and nuclear data uncertainty estimation. In this study, all of the presenting participants mentioned the use of roughly a dozen BFS benchmarks (MIX-MISC-MIXED-001 from ICSBEP) that were used in predicting the MOX application bias and uncertainty.

Nicolas Leclaire (IRSN) presented some preliminary results using the Moret5 code to produce nuclear data sensitivity profiles and using the Scale6.2 Tsunami-ip and Tsurfer sequences to select benchmarks and estimate bias and uncertainty in the application cases. It was noted that using the BLO low-fidelity 44-group covariance data produced a higher prior uncertainty in the applications as compared to the newer 56-group covariance data from ENDF/B-VII.1. While this was expected, the posterior uncertainties in the application cases were insensitive to the covariance data used.

Chris Perfetti (ORNL) discussed many results from various bias prediction methodologies. First, he discussed using USLstats and trending on the benchmark-application correlation coefficients to compute the USL. Using either the 44-group or 56-group covariance data resulted in a very similar USL. Second, he discussed his implementation of the Whisper methodology (using Extreme Value Theory) to compute the USL. While his implementation of the Whisper methodology was similar to the actual implementation in the LANL Whisper code, it wasn't exactly the same. Overall, he concluded that the Whisper methodology was more conservative than the other methods presented, which is likely a valid conclusion in the context of this work. Third, he presented results using the Tsurfer nuclear data assimilation tool in the Scale6.2 code. This final approach was the least conservative of methods presented, but he concluded with a list of open questions regarding finding any experimental outliers and correlations as well as a question about the fidelity needed within the covariance data.

During the phase V presentations, Brown and Rising (LANL) were very active in the discussions of the methodologies and results, and expressed high interest in participating in this phase of the EG. Note that since this meeting (and some before), Rising has been working on using the MCNP6/Whisper tools on these MOX applications in an effort to provide results to the phase V organizers. Ultimately, it will be very beneficial to LANL and the other participants if we remain involved in this study of overall code and bias/uncertainty prediction methods.